

Total Variance: a Progress Report on a New Frequency Stability Characterization*

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Abstract

We give results of recent work on a newly developed frequency stability characterization, called Total variance, whose main advantages are improved confidence at and near the longest averaging time of half the data duration, and lower sensitivity to drift removal. Properties given here, for the standard FM noise types, include mean, degrees of freedom, frequency response, and empirical distribution function.

1 Introduction and Conclusions

This paper is about characterizing common, difficult to characterize frequency noise modulations found at long-term averaging time τ in the output signal of many laboratory frequency standards. It assumes a familiarity with the Allan variance and its characterizations of white, flicker, and random walk FM noise models (WHFM, FLFM, and RWFM) [1].

A shortfall of the currently recommended [2] Allan variance for τ , denoted here by $Avar(\tau)$, is that the usual estimators of it are highly variable at large τ [1, 3, 4] and are sensitive to the method of drift removal [5]. We report statistical properties of a new kind of frequency variance, inherently dependent on measurement duration T as well as τ , called Total variance and denoted hereafter by $Totvar(\tau, T)$ (pronounced *tōt'-vār*). We quantify the improvement in the uncertainty on frequency-stability estimation from the use of $Totvar(\tau, T)$ rather than $Avar(\tau)$ in the presence of FM noises. The square root of this variance, called Total deviation and denoted by $Totdev(\tau, T)$ or the recommended [2] notation $\sigma_{y, TOTAL}(\tau)$, can be interpreted like the Allan deviation $\sigma_y(\tau)$, but with improved confidence at long-term τ , as pointed out in earlier papers [6, 7] and quantified in this paper for FM noises. We do not address the important property that $Totvar(\tau, T)$ appears to have considerably less sensitivity to the method of drift removal than $Avar(\tau)$ [8].

The main advantages of $Totvar$ over $Avar$ are improved confidence at and near the longest averaging time of $\tau = T/2$, and lower sensitivity to drift removal. By theory and simulation we have computed its mean, variance, and empirical probability distribution in the presence of the three FM noise types. Variance results are given in terms of equivalent degrees of freedom [9]. In

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the presence of white FM noise modulation, Total variance is an unbiased estimate of the Allan variance for all τ , yet has three degrees of freedom instead of one at $\tau = T/2$. For all three noise types, the mean and edf of Totvar are given by simple exact or empirical formulas. A comparison of the empirical distribution of Totvar($T/2, T$) with the appropriate chi-squared distribution indicates that confidence intervals based on chi-squared levels are conservative.

In the established tradition of time and frequency statistics, frequency stability is described in terms of finite-difference variances that are ensemble or infinite-time averages of stationary, ergodic increments of phase [12, 13, 14]. In particular, the theoretical Allan variance is a number that depends only on τ , while its conventional estimators are random variables that depend on both τ and T , the largest possible τ being $T/2$. Total variance is a random variable that, along with all its properties, inherently depends on both τ and T . Moreover, Total variance can report values beyond the usual Allan variance last- τ value of $\tau = T/2$; its values at $\tau > T/2$ might be used to augment the normal last- τ value of frequency stability reported at $\tau = T/2$.

We compute the frequency response of Total variance as a function of τ by averaging the squares of the Fourier transforms of Total variance sampling functions, and find that it resembles the frequency response of Allan variance. The results of these investigations indicate that Total variance, while it has an interpretation like that of the Allan variance, also has lower variability and less sensitivity to drift removal.

2 Equations for Totvar (τ, T)

The purpose of this section is to give a precise definition of Totvar(τ, T) for an N_x -point time deviation record with sample period τ_0 . In the following description, the indices m, n , and N_x are related to time by $\tau = m\tau_0$, $t = t_0 + n\tau_0$, and $T = N_x\tau_0$, where t_0 is the time origin and without loss may be made equal to 0.

We start with time-deviation data x_n , $n = 1$ to N_x , with normalized frequency deviations $y_n = (x_{n+1} - x_n)/\tau_0$, $n = 1$ to $N_y = N_x - 1$. Extend the sequence $\{y_n\}$ to a new, longer virtual sequence $\{y_n^*\}$ by reflection as follows: for $n = 1$ to N_y let $y_n^* = y_n$; for $j = 1$ to $N_y - 1$ let

$$y_{1-j}^* = y_j, \quad y_{N_y+j}^* = y_{N_y+1-j}. \quad (1)$$

An equivalent operation can be performed on the original time-deviation sequence $\{x_n\}$ to produce an extended virtual sequence $\{x_n^*\}$ as follows: for $n = 1$ to N_x let $x_n^* = x_n$; for $j = 1$ to $N_x - 2$ let

$$x_{1-j}^* = 2x_1 - x_{1+j}, \quad x_{N_x+j}^* = 2x_{N_x} - x_{N_x-j}. \quad (2)$$

This operation, depicted in Figure 1, is called *extension by reflection about both endpoints*. The result of this extension is a virtual data sequence x_n^* , $n = 3 - N_x$ to $2N_x - 2$, having length $3N_x - 4$ and satisfying $y_n^* = (x_{n+1}^* - x_n^*)/\tau_0$, $n = 3 - N_x$ to $2N_x - 3$.

We now define

$$\text{Totvar}(m, N_x, \tau_0) = \frac{1}{2(m\tau_0)^2(N_x - 2)} \sum_{n=2}^{N_x-1} (x_{n-m}^* - 2x_n^* + x_{n+m}^*)^2, \quad (3)$$

for $1 \leq m \leq N_x - 1$, that is, τ can go to $(N_x - 1)\tau_0$ instead of the usual limit of $[(N_x - 1)/2]\tau_0$. The previous notation Totvar(τ, T) is to be regarded as equivalent to (3) with the dependence on τ_0 suppressed. Totvar can also be represented in terms of extended fractional frequency fluctuation averages as

$$\text{Totvar}(m, N_y, \tau_0) = \frac{1}{2(N_y - 1)} \sum_{n=1}^{N_y-1} (\bar{y}_n^*(m) - \bar{y}_{n-m}^*(m))^2, \quad (4)$$

where $\bar{y}_n^*(m) = (x_{n+m}^* - x_n^*) / (m\tau_0)$.

It can be verified that Totvar, like Avar and its estimators, is invariant to an overall shift in phase and frequency; that is, if a first-degree polynomial $c_0 + c_1n$ is added to the original data set x_n , then Totvar does not change.

We expect the Total variance to be applied mostly to long phase records in which the FM noises dominate the PM noises (white and flicker PM). Then, it is convenient for theoretical purposes to approximate Totvar (m, N_x, τ_0) by a continuous-time analog called Totvarc (τ, T) , in which the sum in (3) is replaced by an integral and dependence on τ_0 is eliminated. The time deviation is now a continuous-time process $x(t)$, given for $0 \leq t \leq T$. Extend $x(t)$ to $x^*(t)$ as follows: for $0 \leq t \leq T$ let $x^*(t) = x(t)$; for $0 < u \leq T$ let $x^*(-u) = 2x(0) - x(u)$ and $x^*(T+u) = 2x(T) - x(T-u)$. Then $x^*(t)$ is given for $-T \leq t \leq 2T$. The continuous analog of Totvar is defined by

$$\text{Totvarc}(\tau, T) = \frac{1}{2\tau^2 T} \int_0^T [x^*(t-\tau) - 2x^*(t) + x^*(t+\tau)]^2 dt, \quad (5)$$

for $0 < \tau \leq T$.

The expressions above are quite different from their equivalent Allan variance expressions. Mainly, Totvar (τ, T) reports a value for an interval τ within data length T based on more samples of the second-difference of phase (or first-difference of average frequency) using a rearranged and extended series of the original data series $\{x_n\}$. It does this by a multiple sample on the phase using a larger, virtual set of data which is an odd, or reflected, extension at the beginning and end (left and right) of the original real set. Figure 1 illustrates the extension and, hence, the resulting circular or repeating representation.

Analyzing a larger virtual data set built from the original data set has been a tool in frequency-domain signal processing for many years. An assumption of periodicity replaces the recurrent behavior (in a time-series sense), a consequence of the ergodic principle [15]. In particular, a range of frequency values (Fourier components) from $0 < f < f_h$ can be extended by a mirror reflection through $f = 0$ so that "negative frequencies" are added to an original data set, resulting in $-f_h < f < f_h$. In the context of time-series analysis, rather than doing extensions of the original vector $\{x_n\}$ and applying the straight second-difference, we alternatively can resample within the original vector; see Section 4 for an algorithm that requires no extension of the data array.

3 Totvarc (τ, T) as an Estimator of Avar (τ)

3.1 Mean and Variance

For computing theoretical moments it is convenient to use the continuous-time random variable Totvarc (τ, T) as a surrogate for the discrete-time random variable Totvar (τ, T) , for the same reason that the calculus of integrals and derivatives is less intricate than the calculus of sums and differences. The mean and variance of Totvarc (τ, T) in the presence of the three standard power-law FM noises were computed by the generalized autocovariance method [4] under the assumption of Gaussian, mean-zero second differences of phase; no frequency drift or drift removal is allowed. The mean $E[\text{Totvarc}(\tau, T)]$ is compared to Avar (τ) ; the variance is most conveniently communicated through the equivalent degrees of freedom (edf), defined for a random variable V by

$$\text{edf}(V) = \frac{2(EV)^2}{\text{var}(V)}. \quad (6)$$

The results, some of which are exact and some of which are empirical fits to numerically computed results, can be expressed as

$$\frac{E[\text{Totvar}(\tau, T)]}{\text{Avar}(\tau)} = 1 - a\frac{\tau}{T}, \quad 0 < \tau \leq \frac{T}{2}, \quad (7)$$

$$\text{edf}[\text{Totvar}(\tau, T)] = b\frac{T}{\tau} - c, \quad 0 < \tau \leq \frac{T}{2}, \quad (8)$$

where a , b , and c are given in Table I. These results were checked by simulations of Totvar (m, N_x, τ_0), with $N_x = 101$.

Table I. Values of a , b and c for FM noises

Noise	a	b	c
WHFM	0	3/2	0
FLFM	$1/(3 \ln(2))$	$24 (\ln(2)/\pi)^2$	0.222
RWFM	3/4	140/151	0.358

The simple, exact form (7) for the mean of Totvar can be interpreted as a scaling property of power-law noise. It turns out this way because the shapes of the sample functions for Totvar and Avar (see Section 4) depend only on τ . For $T/2 < \tau \leq T$ the sampling function shapes depend also on T ; yet, it is noteworthy that (7) persists all the way to T , but only for white FM and random walk FM. The edf results are empirical, with an observed error below 1.2% of numerically computed values; for white FM, though, the edf result appears to be exact, although this is unverified.

For white FM noise processes, Total Variance is an unbiased estimate of the traditional Allan Variance (square of frequency change vs. τ) for all averaging times (τ 's). Its primary advantage, as surmised from (8) and Table I, is a considerable improvement in the confidence of that estimate at longer averaging times. For example, 10 000 seconds of frequency measurements means that τ can't go beyond 5000 seconds ($T/2$) to get one single estimate of frequency-change over the data duration (last half minus first half) using Avar. The edf result (8) for white FM yields the equivalent of three independent estimates ($\text{edf} = 3$) by using Totvar and its multi-sampling function, which is discussed in the next section. The improvement of edf in the presence of FLFM and RWFM (2.097 and 1.514, respectively) is not as dramatic, but substantial nevertheless. For $\tau = T/4, T/8$, etc., the confidence measures of Allan and Total confidence approach each other, until they are essentially the same at $T/16$. For small values of τ/T , the time-deviation record is extended only a short distance at both ends, and hence Totvar (τ, T) differs little from the fully overlapped estimator of Avar (τ) [9].

3.2 Distribution Functions

In the tradition of time and frequency statistics, it is customary to derive confidence intervals for frequency stability on the basis of the assumption that the probability distribution of a frequency stability estimator V , when scaled appropriately, follows the chi-squared distribution with the same edf as V ; see [9]. The chi-squared assumption has been investigated in a limited way for conventional estimators of Allan variance [10, 11]; in view of the greater complexity of Total variance, some investigation of its distribution is appropriate.

Let V denote the Totvar estimator of Allan variance σ^2 , for some τ , and let $r = E(V)/\sigma^2$, $\nu = \text{edf}(V)$, which are presumed known from the previous results. Then the random variable

$$X = \frac{\nu V}{r \sigma^2}$$

has the same mean and edf as does a χ_ν^2 , namely, ν . If X had the χ_ν^2 distribution, then one could derive confidence intervals for σ^2 based on one observation of V .

We carried out a brief investigation of the chi-squared assumption for the most important case of $\tau = T/2$. One thousand independent trials of Totvar(50, 101) were simulated for the three FM noise types, and the empirical distribution functions of X were plotted along with the theoretical chi-squared distribution functions. The chi-squared distributions were good fits to the empirical distributions except at the lower tails, expanded views of which are shown in Figure 2. The empirical tail always lies below the chi-squared tail. Thus, for a probability $p \leq 0.2$, if $x_\nu(p)$ is the chi-squared level for p , and $x_\nu^*(p)$ the level of the scaled Totvar X , we have $x_\nu(p) < x_\nu^*(p)$. Because the upper end of a true confidence interval for σ^2 is proportional to $1/x_\nu^*(p)$ for an appropriate value of p , using $x(p)$ for this purpose gives a conservative confidence interval. For example, suppose we want a 90% confidence interval for σ^2 at $\tau = T/2$ based on $V = \text{Totvar}(T/2, T)$ and a white-FM noise assumption. Then $r = 1$, $\nu = 3$; the 5% and 95% χ_3^2 levels are 0.352 and 7.81; and a 90% confidence interval for σ^2 based on chi-squared is $[3V/7.81, 3V/.352] = [0.384V, 8.52V]$. (Take square roots for σ .) The more realistic value of 0.60 for the 5% Totvar level from Figure 2(a) reduces the upper end of the confidence interval to $5V$.

4 Sampling Functions and Frequency Responses

Extending by reflection an original $\{x_n\}$ vector at both ends and then applying a second difference can be equivalently represented as four different types of differencing on $\{x_n : n = 1, \dots, N_x\}$ directly. The summand of Totvar(m, N_x, τ_0) in the following equation takes on four forms that depend on the relationship of n to a given m and N_x :

$$\text{Totvar}(m, N_x, \tau_0) = \frac{1}{2(m\tau_0)^2(N_x - 2)} \sum_{n=2}^{N_x-1} D_n^2, \quad (9)$$

where

$$\begin{aligned} D_n &= x_{n-m} - 2x_n + x_{n+m} & : & \quad m - n \geq 1, \quad m + n \leq N_x, \\ D_n &= 2x_1 - x_{2-n+m} - 2x_n + x_{n+m} & : & \quad m - n < 1, \quad m + n \leq N_x, \\ D_n &= x_{n-m} - 2x_n + 2x_{N_x} - x_{2N_x-n-m} & : & \quad m - n \geq 1, \quad m + n > N_x, \\ D_n &= 2x_1 - x_{2-n+m} - 2x_n + 2x_{N_x} - x_{2N_x-n-m} & : & \quad m - n < 1, \quad m + n > N_x. \end{aligned}$$

We can derive from these expressions the frequency sampling functions associated with Totvar(τ, T), that is, how its terms act on $y_n = (x_n - x_{n-1})/\tau_0$, and contrast them with the simpler sampling function associated with Avar(τ) (see Figure 3), which gives the change in average frequency from one τ interval to the next [7]. The augmentation incorporated in Totvar(τ, T) combines the sequential sampling function with others, which makes its sampling technique bizarre, but nevertheless shown in Figure 4.

Although the time-domain presentation of the action of Totvar on frequency residuals seems to give little insight, we can use the Fourier transform of these sampling functions to derive frequency responses that perhaps convey more meaning. The continuous analog version of Totvar(τ, T) can be written in the form

$$\text{Totvarc}(\tau, T) = \frac{1}{2\tau^2 T} \int_0^T dt \left[\int_0^T du y(u) h_y(u; t, \tau) \right]^2, \quad (10)$$

where $h_y(u; t; \tau)$ is the sampling function for $\nabla_{\tau}^2 x^*(t)$ (for the extended $x^*(\cdot)$ record) in terms of $y(u) = dx(u)/du$, $0 < u < T$. Let $H_y(f; t, \tau) = \int_0^T h_y(u; t, \tau) e^{-i2\pi f u} du$. We can show that the expected value is given in terms of $S_y(f)$, the one-sided spectral density of $y(t)$, by

$$E[\text{Totvarc}(\tau, T)] = \int_0^{\infty} W_y(f; \tau, T) S_y(f) df, \quad (11)$$

where

$$W_y(f; \tau, T) = \frac{1}{2\tau^2 T} \int_0^T |H_y(f; t, \tau)|^2 dt. \quad (12)$$

$W_y(f; \tau, T)$ can therefore be regarded as the mean frequency response of Totvar as an action on $y(t)$. Figure 5 shows this frequency response plotted against $f\tau$ for $\tau/T = 0.1, 0.2, \dots, 0.5$. The frequency response of Allan variance (dotted curve) is the limit of Totvar response as $\tau/T \rightarrow 0$. Also shown (dashed curve) is the frequency response of $2 \cdot \text{Totvarc}(T, T)$, regarded as an estimator of $\text{Avar}(T/2)$ (see Section 5 below).

$\text{Totvarc}(\tau, T)$ has an approximate Allan-like response; more importantly, Totvar does not have the deep nulls encountered with $\text{Avar}(\tau)$ near $\tau = T/2$; consequently it has less variability and hence better confidence as indicated by an increased edf. We showed that the estimate (*vis-à-vis* $E[\text{Totvarc}(\tau, T)]$) is an unbiased estimate of $\text{Avar}(\tau)$ for WHFM noise and slightly biased for FLFM and RWFM noise. This may be somewhat evidenced by noting the slight reduction in the amplitudes of the main lobes of the frequency responses in Figure 5.

5 Properties of $\text{Totvarc}(T, T)$

Although we have defined Totvar for τ all the way up to $(N_x - 1)\tau_0$, we can realistically expect to obtain meaningful frequency stability results only $\tau \leq T/2$. Nevertheless, we computed the mean and edf of $\text{Totvarc}(\tau, T)$ for $T/2 < \tau \leq T$. For white and random walk FM, *twice* $\text{Totvarc}(T, T)$ is unbiased for $\text{Avar}(T/2)$ and is almost unbiased (within a factor of $2/(3 \ln(2)) = 0.9618$) for flicker FM. This result was motivated by comparing the frequency responses of $2 \cdot \text{Totvarc}(T, T)$ and $\text{Avar}(T/2)$, as seen in Figure 5. Unfortunately, $\text{Totvarc}(T, T)$ has a smaller edf (1.5, 1.126, and 1.029 for WHFM, FLFM, and RWFM) than $\text{Totvarc}(T/2, T)$ does, and hence the mean-squared error (bias² + variance) of $2 \cdot \text{Totvarc}(T, T)$ as an estimator of $\text{Avar}(T/2)$ is greater than that of $\text{Totvarc}(T/2, T)$, so we might still prefer $\text{Totvarc}(T/2, T)$, or perhaps some linear combination of the two. This possibility has yet to be investigated, but other work indicates that Total variance coefficients beyond $\tau = T/2$ could justifiably be incorporated in the last $T/2$ value usually reported. Summing all the familiar "power-of-2" τ -values in a Total variance plot leads to exactly twice the standard sample variance, much in the same way that integrating an estimate of a spectrum also yields the sample variance [18].

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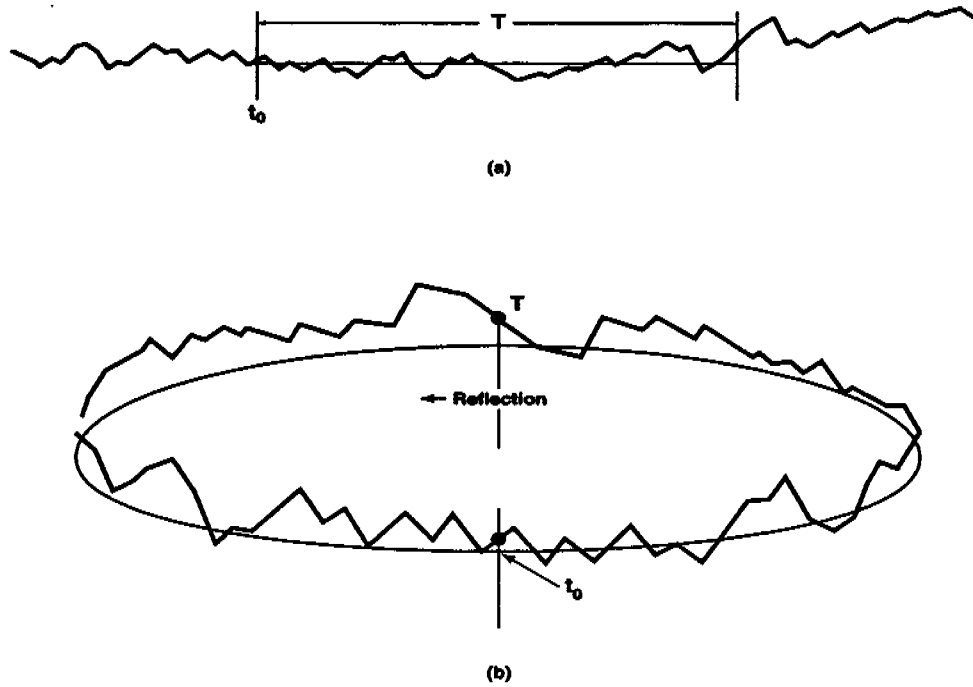


Figure 1: (a) Extension of a phase record by reflection at both ends; (b) circular representation of extended phase record

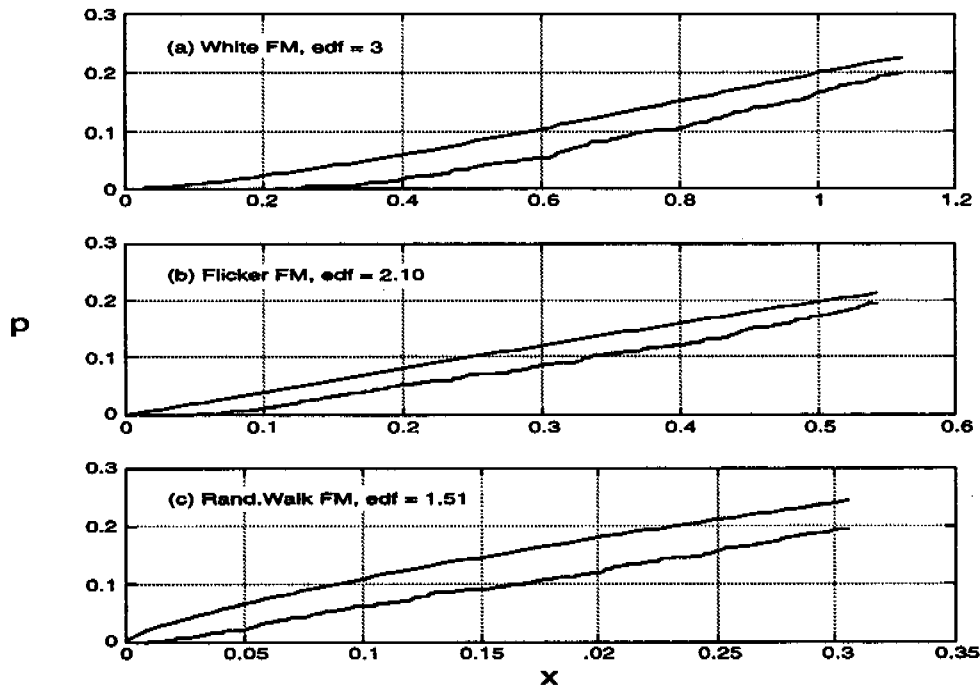


Figure 2: Expanded views of the lower tails of empirical Totvar distribution functions (lower curves), and the corresponding chi-squared distribution functions (upper curves)

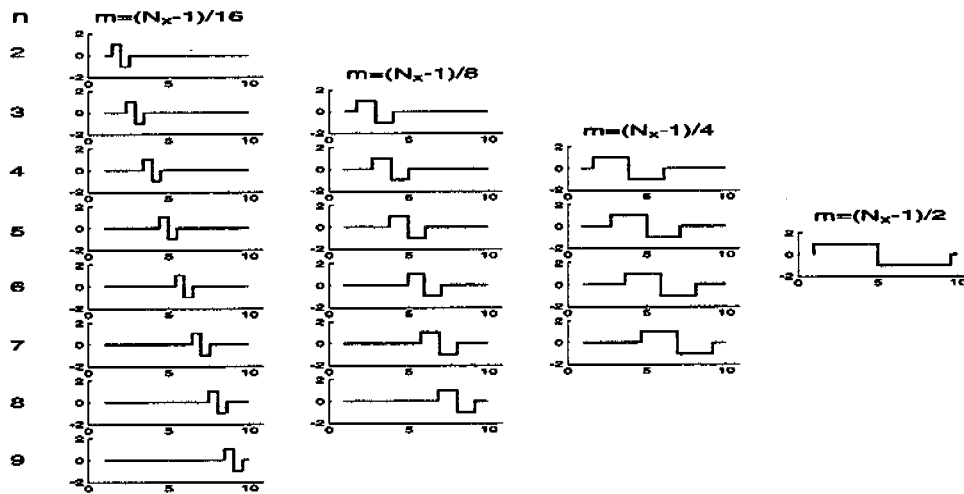


Figure 3: Usual sampling given by Avar for values of m and n when $N_x=10$, $m \leq (N_x - 1)/2$

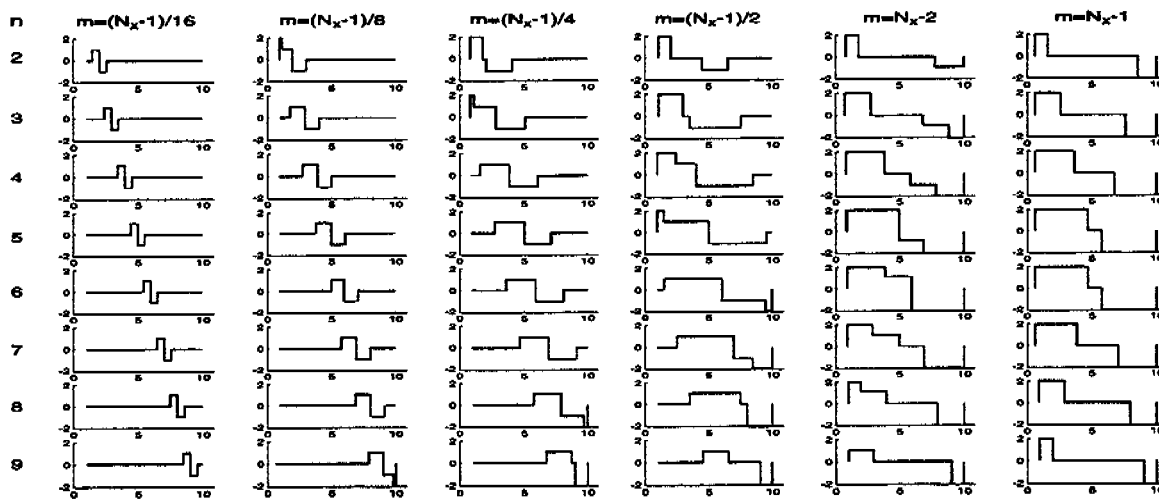


Figure 4: Sampling given by Totvar for values of m and n when $N_x=10$; note that m is not restricted to $m \leq (N_x - 1)/2$ as with Avar

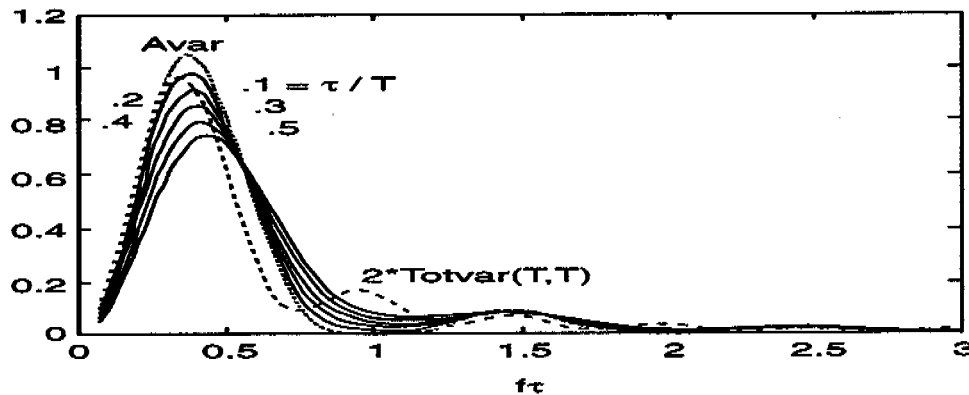


Figure 5: Mean frequency responses of Avar and Totvar as operations on $y(t)$

Questions and Answers

CLAUDINE THOMAS (BIPM): If we want to use the total variance, we must first be sure that there is no frequency drift in the data.

DAVE HOWE (NIST): Oh, that is not true. We no longer have to remove the drift or some coefficient, at any rate. We never know the drift in real data; in simulation we, of course, can –

CLAUDINE THOMAS: But, when you circle the data, if you have a frequency drift, of course, you will have an offset.

DAVE HOWE: Well, no. As a matter of fact – let me put that slide back on here, that is a very good question. I will put this up. This is the original data, this is 20 simulations of random walk FM. So the data duration extends with Index 1 to 1025. The procedure calls for extending that at both ends. So, the vector that you actually work on is going to look like that.

Now, in the presence of drift, because it is a mirrored reflection, if there is a trend in the data at the adjoint, when you are adding or extending the data set, then there will not be any discontinuity by taking the second difference. Yes, you have to think about it a little bit, but what we do is we actually reverse the data set and we also mirror it. So, even if there is a racing trend through that last point, or the first point, then there's no discontinuity in looking at the variance, which would be the second difference in that.

CLAUDINE THOMAS: Thank you for your answer. I also have another question. Does the use of the total variance suppose that your system is more or less stationary; that at the beginning and the end of the Tau, of the big T lines, the statistical properties of the system should be the same? Because, when you circle, the statistical properties are completely different. I am thinking about the total time scale of course.

DAVE HOWE: Yes. First of all, by construction, we have a situation where the variance for the original data has to be the same as the variance for the extended data, and that again is by construction. We have not added any additional data; we are using the original data; and constructed it in a way that added more terms, what we call "surrogate terms," which will contribute to the answer that you get in the long term. Nevertheless, getting back to your remark about circularizing the data –

CLAUDINE THOMAS: My question was you have a span of data –

DAVE HOWE: The treatment that we apply does not have any restriction regarding stationarity.